

Fine-structure in the infrared OH-stretching bands in orthorhombic amphiboles of holmquistite and anthophyllite-gedrite series

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The principal infrared OH-stretching bands in the Pnma orthorhombic Mg-Fe-Mn-Li amphiboles holmquistite and anthophyllite show fine structure due to the occurrence of two symmetrically distinct OH groups in the crystal structure. There are two distinct tetrahedral double-chains in the orthorhombic amphibole structure, the A-chain and the B-chain. The B-chain is more rotated than the A-chain, and the stereochemistry around each of the OH sites suggests that the hydrogen bond to the bridging anion(s) of the B-chain is stronger than the hydrogen bond to the bridging anion(s) of the A-chain. This difference is sufficient to shift the frequency of the principal OH₂ stretching band(s) ~5 cm⁻¹ to lower frequency, and allows resolution of the two bands in the infrared spectrum. This distinction could allow detection of possible OH, F ordering between the two distinct monovalent-anion sites in the orthorhombic amphibole structure.